

Synthesis and Characterization of an Open-Framework Copper- Germanium Phosphate $[\text{Cu}(\text{H}_2\text{O})_2(\text{OH})]_2\text{Ge}(\text{PO}_4)_2$ [†]

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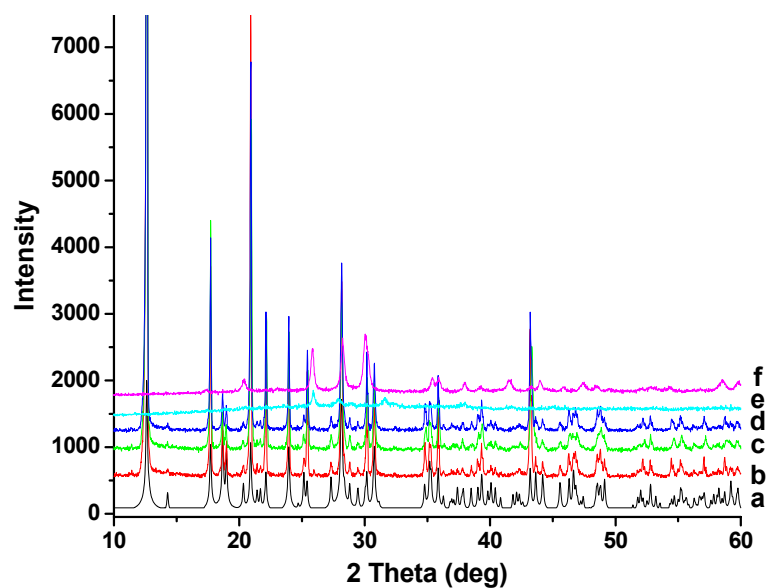


Figure S1. Powder XRD diagrams (Philips X'pert X-ray diffractometer using Cu-K α radiation, $\lambda = 1.5418\text{\AA}$) for (a) the simulated, (b) as-synthesized, and calcined NJU-1 at (c) 150, (d) 200, (e) 250, and (f) 700°C, respectively, for 2 h with a ramp rate of 1°C/min.

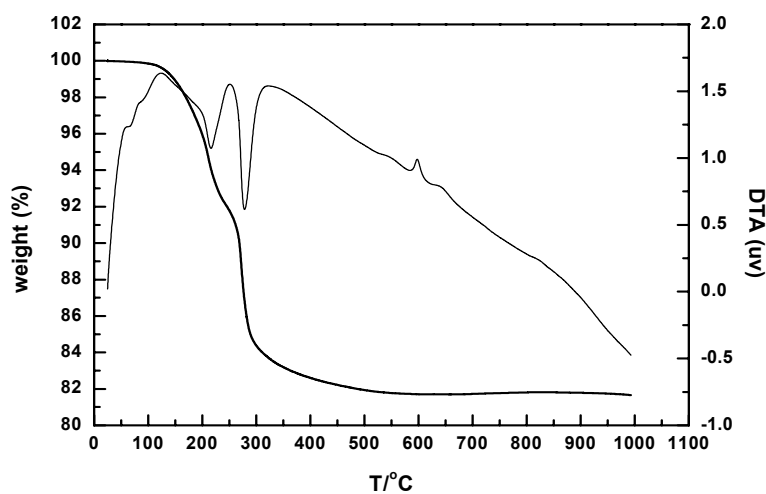


Figure S2. TG-DTA profiles for NJU-1 in N₂ (flow rate of 100 ml min⁻¹) with a ramp rate of 10°C/min.

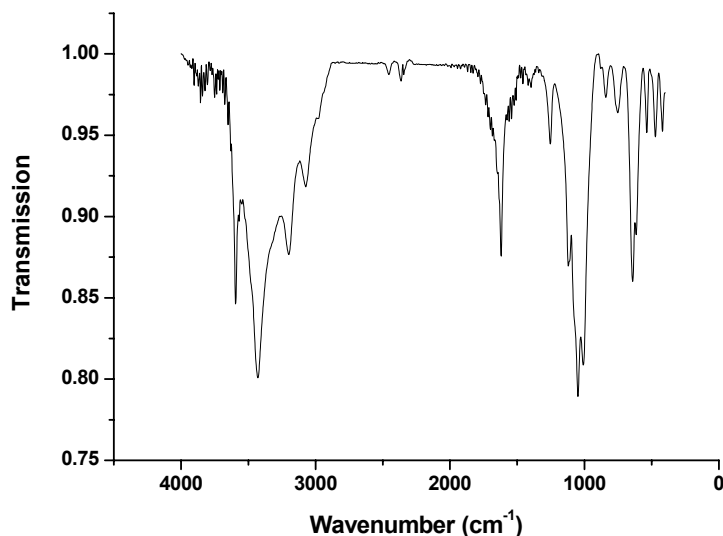


Figure S3. FT-IR spectrum for NJU-1 (KBr pellet).

Magnetic data analysis

The magnetic susceptibility measurement of $\text{Cu}_2\text{GeH}_{10}\text{O}_{14}\text{P}_2$ was performed on the Quantum Design MPMS-XL7 SQUID magnetometer at temperatures ranging from 1.8 to 300 K. The data were fitted as 1D uniform antiferromagnetic chains of $S = 1/2$ spins based on the spin Hamiltonian, $H = -J\sum S_i S_{i+1}$. According to Bonner and Fisher the molar susceptibility is given by

$$\chi = \frac{Ng^2\beta^2}{kT} \frac{0.25 + 0.074975x + 0.075235x^2}{1.0 + 0.9931x + 0.172135x^2 + 0.757825x^3} \quad \text{and } x = |J|/kT$$

where N is Avogadro's number, β is Bohr magneton, k is the Boltzmann constant, J is the exchange coupling constant describing the magnetic interaction between any two adjacent unit with an $S = 1/2$ spin. The fitting parameters for $\chi_M T$ versus T are $g = 2.07$, $-J = 2.05 \text{ cm}^{-1}$, $R = 7.1 \times 10^{-3}$ (defined as $\sum[(\chi_M T)_{\text{calc}} - (\chi_M T)_{\text{obs}}]^2 / \sum[(\chi_M T)_{\text{obs}}]^2$). The negative J values indicate that weak antiferromagnetic coupling between Cu^{II} ions bridged by water molecules.